



IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

H8  
Plunkett  
5/7/02

Applicants: Michael Pitman, et al Docket No.: YOR919980112

Serial No.: 09/275,568

Group Art Unit: 1631

Filed: March 24, 1999

Examiner: Sheinberg, Monika B.

For: Similarity Searching of Molecules Based upon Descriptor  
Vectors Characterizing Molecular Regions

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MAY 03 2002

**INFORMATION DISCLOSURE STATEMENT**

TECH CENTER 1600/2900

The Commissioner of Patents and Trademarks  
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Arlington, Va 22202

Sir:

In order to assist in the examination of this application, and in accordance with 37 CFR 1.56, 1.97 and 1.98, copies of the documents listed on the attached form PTO-1449 are forwarded herewith.

By:

Attorney: Manny W. Schecter

Reg. No.: 31,722

(914) 945-3252

IBM Corporation  
Intellectual Property Law Dept.  
P. O. Box 218  
Yorktown Heights, New York 10598

FORM PTO-1449 (Modified)

ATTY. DOCKET NO.

SERIAL NO.

YOR919980112

09/275,568

LIST OF PATENTS AND PUBLICATIONS  
FOR APPLICANT'S INFORMATION  
DISCLOSURE STATEMENT

APPLICANT: Michael C. Pitman, et al

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## REFERENCE DESIGNATION

## U.S. PATENT DOCUMENTS

EXAMINER INITIALS		DOCUMENT NUMBER	DATE	NAME	CLASS	SUBCLASS	FILING DATE (IF APPRO.)
	AA	5,025,388	06/18/91	Cramer et al			
	AB	5,784,294	07/21/98	Platt et al			
	AC						
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## FOREIGN PATENT DOCUMENTS

		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUBCLASS	TRANSLATION	
							YES	NO
	AL							
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	AN							
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## OTHER ART (Including Author, Title, Date, Pertinent Pages, etc.)

AQ	Perkins et al., "Molecular surface-volume and property matching to superpose flexible dissimilar molecules." J. Comput.-Aided Mol. Des. 1992, Vol 6, pp. 475-486
AR	Willet et al., "Similarity Searching in Files of Three-Dimensional Chemical Structures: Flexible Field-Based Searching of Molecular Electrostatic Potentials." J. Chem. Inf. Comput. Sci. 1996, Vol 36, pp. 900-908
AS	Gerhard Klebe, "Structural Alignment of Molecules." Klebe, G., Structural Alignment of Molecules, in 3D QSAR in Drug Design. Theory, Methods and Practice, pp 173-199
AT	Press et al., "Numerical Recipes." Cambridge University Press, 1986, pp 349-363.
AU	Richard D. Cramer et al., "Comparative Molecular Field Analysis (CoMFA). 1. Effect of Shape on Binding of Steroids to Carrier Proteins. J. Am. Chem. Soc. Vol. 110, 1988, pp. 5959-5967

EXAMINER

DATE CONSIDERED

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to applicant.

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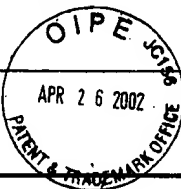
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## OTHER ART (Including Author, Title, Date, Pertinent Pages, etc.)

AW	Andrew C. Good et al., "Structure-Activity Relationships from Molecular Similarity Matrices." J. Med. Chem., Vol. 36, 1993, pp. 433-438
AX	Ajay N. Jain et al., "Predicting Biological Activities from Molecular Surface Properties. Performance Comparisons on a Steroid Benchmark." J. Med. Chem., Vol. 37, 1994, pp. 2315-2327.
AY	William Fisanick et al., "Similarity Searching on CAS Registry Substances. 1. Global Molecular Property and Generic Atom Triangle Geometric Searching." Journal of Chemical Information & Computer Sciences, Vol. 32, No. 6, 1992, pp 664-674
AZ	William Fisanick et al., "Similarity Searching on CAS Registry Substances. 2. 2D Structural Similarity." Journal of Chem Info & Computer Sciences, Vol. 34, No. 1, 1994, pp 130-140
BA	Ken Turkowski, "The Use of Coordinate Frames in Computer Graphics." Academic Press, edited by A. Glassner, pp 522-532

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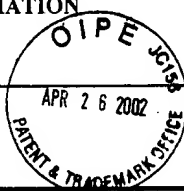
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## OTHER ART (Including Author, Title, Date, Pertinent Pages, etc.)

BB	Michael L. Connolly, "Computation of Molecular Volume." JACS, Vol. 107, 1985, pp 1118-1124
BC	Mike Crenshaw Pitman, "Fragment Assembly in the Automated Molecular Invention system: Invention by Mike Crenshaw Pitman, 1995, University of California, Santa Cruz, pp 1-199
BD	Yvonne C. Martin, "A Fast New Approach to Pharmacophore Mapping and its Application to Dopaminergic and Benzodiazepine Agonists", J. Comput.-Aided Molecular Design, 1992, Vol. 6, pp 83-102
BE	
BF	

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